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CONFORMATION AND ANISOTROPY OF CHEMICAL BONDS IN CYCLIC ETHERS INVESTIGATED BY N.M.R. SPECTROSCOPY

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In the given work conformations of cyclic ethers of carbonic and sulphureous acids of 2.2-dimethylpropandiol-1.3, propandiol-1.3 and ethandiol-1.2 have been studied. Part of n.m.r spectra of protons (PMR) is shown in Fig. 1. The spectra (a,b,d) were obtained using n.m.r. spectrometer operating at 24.46 Mc/s[1] at resolution of 5 parts in 10^8 got by means of Anderson's shims[2], spectrum (c) attained by JNM-3 high-resolution spectrometer.

In PMR spectrum of 2.2-dimethylpropandiol-1.3 carbonate (a) a wide methylene peak showing an unresolved multiple structure with a chemical shift τ=6.13±0.04 p.p.m. (4) and the peak of methyl groups with τ=9.03±0.04 p.p.m. (6)+ may be found. The crystals of the compound were dissolved in CCl_4 at concentration of ~35%. The sulphite spectrum (b) consists a methylene quartet the centre of which has τ=6.17 p.p.m. (4) and a methyl duplicate with the centre τ=9.09 p.p.m. (6). Unresolved multiplicity may be found in each peak of the quartet arising from indirect spin-spin interaction with CH_3 group. The sulphite sample was degassed by means of repeatedly freezing, pumping out till 10^{-3} mm Hg and defreezing again.

The fact that we have a striking difference in the spectrum of carbonite and that of sulfite is explained by conformations of cyclic ethers. It is well known that the CO_3 group of carbonic acid derivatives is flat whereas the SO_3group of sulphureous acid derivatives is pyramidal[3]. The conformational formulars carbonite and sulfite see Fig. 1. Thanks to the flat structure of CO_3 group the transition of one form of the chaire into the other gives an equivalent structure. If it is sulphite both conformational forms

+ The brackets show relative integral intensivity of the lines.

1 Yu.Yu. Samitov, Prib. i techn. exper. (U.S.S.R.), N5, 100 (1961).

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